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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/573,023	03/22/2006	Yasuhige Yonezawa	W 1878.0229.	4509
32172	7590	04/17/2008	EXAMINER	
DICKSTEIN SHAPIRO LLP			BORIN, MICHAEL L	
1177 AVENUE OF THE AMERICAS (6TH AVENUE)			ART UNIT	PAPER NUMBER
NEW YORK, NY 10036-2714			1631	
			MAIL DATE	DELIVERY MODE
			04/17/2008	PAPER

**Please find below and/or attached an Office communication concerning this application or proceeding.**

The time period for reply, if any, is set in the attached communication.

<b>Office Action Summary</b>	<b>Application No.</b>	<b>Applicant(s)</b>
	10/573,023	YONEZAWA ET AL.
	<b>Examiner</b>	<b>Art Unit</b>
	Michael Borin	1631

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

#### Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 1 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

#### Status

1) Responsive to communication(s) filed on \_\_\_\_\_.  
 2a) This action is **FINAL**.                    2b) This action is non-final.  
 3) Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

#### Disposition of Claims

4) Claim(s) 1-18 is/are pending in the application.  
 4a) Of the above claim(s) \_\_\_\_ is/are withdrawn from consideration.  
 5) Claim(s) \_\_\_\_ is/are allowed.  
 6) Claim(s) \_\_\_\_ is/are rejected.  
 7) Claim(s) \_\_\_\_ is/are objected to.  
 8) Claim(s) 1-18 are subject to restriction and/or election requirement.

#### Application Papers

9) The specification is objected to by the Examiner.  
 10) The drawing(s) filed on \_\_\_\_ is/are: a) accepted or b) objected to by the Examiner.  
 Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).  
 Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).  
 11) The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

#### Priority under 35 U.S.C. § 119

12) Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).  
 a) All    b) Some \* c) None of:  
 1. Certified copies of the priority documents have been received.  
 2. Certified copies of the priority documents have been received in Application No. \_\_\_\_\_.  
 3. Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

\* See the attached detailed Office action for a list of the certified copies not received.

#### Attachment(s)

1) Notice of References Cited (PTO-892)  
 2) Notice of Draftsperson's Patent Drawing Review (PTO-948)  
 3) Information Disclosure Statement(s) (PTO/SB/08)  
 Paper No(s)/Mail Date \_\_\_\_\_.  
 4) Interview Summary (PTO-413)  
 Paper No(s)/Mail Date \_\_\_\_\_.  
 5) Notice of Informal Patent Application  
 6) Other: \_\_\_\_\_.

## DETAILED ACTION

Claims 1-18 are pending.

### *Election/Restrictions*

Restriction is required under 35 U.S.C. 121 and 372.

This application contains the following inventions or groups of inventions which are not so linked as to form a single general inventive concept under PCT Rule 13.1.

In accordance with 37 CFR 1.499, applicant is required, in reply to this action, to elect a single invention to which the claims must be restricted.

Group I, claim(s) 1 and 3-6,14,15 (in part), drawn to molecular simulation method for dividing a molecule or a part of molecule to be simulated into a QM space and an MM space by replacing a part of a total energy expression in the ab initio molecular orbital method concerning the QM space with an empirical potential.

Group I, claims 2 and 3-6,14,15 (in part), drawn to molecular simulation method for dividing a molecule or a part of molecule to be simulated into a QM space and an MM space by replacing a part of the total energy expression concerning the superficial QM region with a term based on the empirical potential; and obtaining total energy in the ab initio molecular orbital method concerning the QM space

Group III, claim(s) 8-10,16,17, drawn to molecular simulation device, and claims 11,12, 13,18, drawn to corresponding computer program and storage medium.

The inventions listed as Groups I-III do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Group I is the technical feature that links Groups I-III. Group II is not the contribution over the prior art because it is suggested by references teaching semi-empirical QM/MM molecular simulation methods. For example, such methods are in Field et al, or Reuter et al., or Bessac et al. Therefore, the lack of unity is present because the linking technical feature is not a “special technical feature” as defined by PCT Rule 13.2.

The method of Group I does not require creating superficial QM region and using a term that is based on empirical potential. Nor the method of Group I requires obtaining total energy in the ab initio molecular orbital method concerning the QM space.

The particular molecular simulation device, and corresponding computer program and storage medium are not required for method of Group I. With respect to method of Group II, the method can be carried out without the device of Group III, e.g., manually.

Because these inventions are distinct for the reasons given and have acquired a separate status in the art because of their recognized divergent subject matter, restriction for examination purposes as indicated is proper.

If applicant elects claims directed to the product, and a product claim is subsequently found allowable, withdrawn process claims which depend from or otherwise include all the limitations of the allowable product claim will be rejoined. (MPEP 821.04)

Applicant is advised that the response to this requirement to be complete must include an election of the invention to be examined even though the requirement be traversed (37 CFR 1.143).

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Michael Borin whose telephone number is (571) 272-0713. The examiner can normally be reached on 9am-5pm.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Marjorie Moran can be reached on (571) 272-0720. The fax phone number for the organization where this application or proceeding is assigned is 571-273-8300.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see <http://pair-direct.uspto.gov>. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free). If you would like assistance from a USPTO Customer Service Representative or access to the automated information system, call 800-786-9199 (IN USA OR CANADA) or 571-272-1000.

/Michael Borin, Ph.D./  
Primary Examiner, Art Unit 1631